The High Energy-Density instrument at the European XFEL



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Science case

The science scope of the HED instrument focuses on states of matter at high density, temperature, pressure, electric and/or magnetic field. Major applications are highpressure planetary physics, warm- and hot- dense matter, laser-induced relativistic plasmas and complex solids in pulsed magnetic fields. These extreme states can be reached by different types of optical lasers, the X-ray FEL beam and pulsed coils. User operation at the HED instrument is foreseen to start in Q2 2019.

Properties of XFEL undulator for HED (SASE2)		X-ray diagnostics available at HED	
SASE2 undulator		X-ray diffraction	
Hard X-ray source	3 – 25 keV photon energy, 10 ⁻³ SASE bandwidth, 10 ⁻⁵ self-seeded	nergy, 10 ⁻³ SASE bandwidth, 10 ⁻⁵ self-seeded IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII	
Repetition rate	10 Hz bunch trains with up to 2700 pulses	IC1 and IC2: large area detectors in air (or in air pocket in vacuum): Perkin-Elmer	
Pulse energy 10 ⁸ – 10 ¹³ X-ray photons per pulse / 100 nJ – few mJ GaAs AGIPD on detector bench with central hole (220-ns framing to record bunch patter)		GaAs AGIPD on detector bench with central hole (220-ns framing to record bunch pattern)	
Pulse duration	2 to 100 fs (correlates with bunch charge)	Inelastic X-ray scattering	
UED instrument V rov ention 8 has a characteristics		Two HAPG von-Hamos spectrometers ($\Lambda E < 9 \text{ eV}$) on motorized rails on vertical breadboard	

HED instrument X-ray optics & beam characteristics

- □ Three mirrors (two for beam offset & one for distribution between HED / MID instruments)
- □ Monochromators: 4-bounce Si_{111} (5 25 keV, ~10⁻⁴), high-resolution monochromator (~10⁻⁶)
- **G** Focusing: Be lenses at three positions (229, 857 and 962 m downstream of the undulator exit) resulting in spot sizes of ~200 μ m, ~20 μ m, and 1 – 3 μ m FWHM for 5 – 25 keV
- □ Split & Delay Line (BMBF project, U Münster): Delays: ~2 ps (20 keV) to ~23 ps (5 keV) **Repetition rate**
- \Box 4.5 MHz, 1 10 Hz, shot-on-demand

- APG von-mattices spectrometers ($\Delta E > 9 ev$) on motorized rails on
- Spherical diced Si (533) analyzers for $E/\Delta E \sim 10^{-6}$ high resolution inelastic x-ray scattering

X-ray absorption spectroscopy

- Bent Si crystal spectrometers before IC1. Future plan to built a second one after interaction point. SAXS, PCI, ...
- Placed on detector bench

Emission spectroscopy

□ Flexible flat and bent perfect crystals coupled to ePIX100 detectors







ePix100 (SLAC)	ePix10k (SLAC)	Jungfrau (PSI)	Gotthard-I (PSI)
300 µm Si	300 µm Si	320 µm Si	320 µm Si
704 × 768 (35×38 mm ²)	352 × 384 (35×38 mm ²)	512 × 1024 (40×80 mm ²)	1 × 1280 (8×64 mm ²)
50	100	75	50
10 ² (@ 8 keV)	10 ⁴ (@ 8 keV)	10 ⁴ (@ 12 keV)	10 ⁴ (@ 12 keV)
~260	~560	~450	~900
120	120	2,000 0.5 MHz in burst mode, 16 images on-chip memory	40,000 0.8 MHz in burst mode, 128 images digital buffer
2	3	4	2
	ePix100 SLAC 300 μm Si 704 × 768 (35×38 mm²) 50 10² (@ 8 keV) ~260 120 2	ePix100 (SLAC)ePix10k (SLAC)300 μm Si300 μm Si704 × 768 (35×38 mm²)352 × 384 (35×38 mm²)5010010² (@ 8 keV)104 (@ 8 keV)~260~56012012023	ePix100 (SLAC)ePix10k (SLAC)Jungfrau (PSI)300 μm Si300 μm Si320 μm Si704 × 768 (35×38 mm²)352 × 384 (35×38 mm²)512 × 1024 (40×80 mm²)501007510² (@ 8 keV)10⁴ (@ 8 keV)10⁴ (@ 12 keV)~260~560~450120120120234



HED Instrument Parameters for Early User Operation

HED

All parameters are subject to change, depending on the commissioning process of both the accelerator and the instrument.

For more information, please contact: ulf.zastrau@xfel.eu

X-Ray Photon Beam Parameters

photon energy	9 keV	Adjustable 7-25 keV
pulse energy	0.5 – 1 mJ	Up to 2 mJ
photons per pulse	3 x 10 ¹¹	Estimated by SPB/SFX, FXE
pulse duration	10 fs	Derived by theory group
spot size on sample	min. 1 µm	Variable up to ~ mm
photons/µm ² on sample	10 ⁹ -10 ¹⁰	Derived by SPB/SFX, FXE
train repetition rate	10 Hz	Fixed
Intra-train repetition rate	1.1, 4.5 MHz	Possibly 100 kHz; arbitrary
No. of bunches per train	1-60	Possibly up to 300
ΔE/E	~ 0.2%	Estimated by SPB/SFX, FXE

Spectrometers (diagnostics and experimental)

Single Shot Spectrometer (CAEP)

Crystals	4x 10 μm Si	
Energy	3-15 keV with grating	5-25 crystal only
Energy resolution (dE/E)	< 1 x 10 ⁻⁴	
Detector	Optical CCD (2D)	Gotthard-I (1D)
Detector arm rotation	30° - 90°	

Experimental (Analyser crystals for IXS and hrIXS)

4 high resolution diced analyzers	Si 533	10 mm diameter, R = 1 m spherical
2 mosaic spectrometers	HAPG 002	R= 50 and 75 mm, cylindrical 32 mm x 30 mm size

Monochromators

High-Energy Density science

X-ray bandwidth

∆ E/E En	ergy
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Detectors

Parameters	ePix100	ePix10k	Jungfrau	Gotthard-I
Farameter 5	GLIVIOO	GLIVIA	Jungnau	Gottilaru-i

European XFEL

	SLAC	SLAC	PSI	PSI
Sensor	300 µm Si	300 µm Si	320 μm Si (upgr 450 μm Si)	320 µm Si
Sensor size (pixel)	704x768 (35x38 mm ²)	352x384 (35x38 mm ²)	512x1024 (40x80 mm ²)	1x1280 (8x64 mm²)
Pixel size (µm)	50	100	75	50
Dynamic range	10 ² (@ 8 keV)	10 ⁴ (@ 8 keV)	10 ⁴ (@ 12 keV)	10 ⁴ (@ 12 keV)
Noise (eV)	<280	<560	<450	<900
Repetition (Hz)	120	120	2,000 *	40,000 **
# of modules	2	3	4	2

* 0.5 MHz in burst mode, 16 images on-chip memory

** 0.8 MHz in burst mode, 128 images digital memory

Split and Delay Unit

X-ray energy	Delay	Multilayers
5 keV	~23 ps	Ni/B₄C (<12 keV)
15 keV	~4 ps	Mo/B₄C (8-20 keV)
20 keV	~2 ps	

SASE	10 ⁻³	3-25 keV
Si ₁₁₁ mono	10 ⁻⁴	5-25 keV
Si ₅₃₃ high-res mono	10 ⁻⁶	7.494 keV

Target delivery

Target system	Samples	Rep rate
High precision positioning system	RMT's, wires, structured targets	Shot on demand
Fast Sample Scanner	Foil, crystal, powder	1 – 10 Hz
Cryogenic jets	Solid H2, D2, HD, CH4, Ne, Ar	10 Hz

Optical Laser Systems*

	λ (nm)	Max repetition rate	Pulse diffraction	Max. pulse energy
PP	~ 800	0.1 – 4.5 MHz	15 – 300 fs fourier-limited	≤ 2 mJ
PP	1030	0.1 – 4.5 MHz	~ 1 ps	≤ 40 mJ
HI (Amplitude)	~ 800	10 Hz	~25 fs	≤ 10 J
HE (DiPOLE)	515 (1030 fundamen tal)	1 – 10 Hz	15 ns or shorter	~100 J at 1030 nm

* Please inquire HED staff about availability

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X-ray beam transport and properties at the **High Energy Density science instrument at European XFEL**

European

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Abstract

The HED science instrument is located at the SASE2 undulator, which produces hard X-rays in an energy range between 3 and 25 keV. The first 390 m downstream of the undulator source are shared with the scientific instrument MID [1]. A distribution mirror is located at 390 m that allows to stir the beam to the HED science instrument which is located in the experimental hall at about 970 m from the source [2, 3, 4]. As additional optical elements we foresee two monochromators, a split and delay unit, a quarter wave plate and four positions for focusing optics in the tunnel and in the experimental hall. This leads to a variety of X-ray beam properties at the sample position, that can be selected for the respective experiment. Major X-ray beam diagnostics in the HED part of the beamline comprise on-line monitoring of the arrival time of X-rays and optical lasers [5], an in-situ single-shot X-ray spectrometer combining a diamond grating with a convex Si crystal following the concept of [6], as well as intensity and position monitors.

XFEL beam properties

SASE2 undulator

Hard X-ray source	3 – 25 keV photon energy, 10 ⁻³ SASE bandwidth, 10 ⁻⁵ self- seeded
Repetition rate Pulse energy Pulse duration	10 Hz bunch trains with up to 2700 pulses, pulse on demand $10^8 - 10^{13}$ X-ray photons per pulse / 100 nJ – few mJ 2 to 100 fs (correlates with bunch charge)

X-ray beam optics and properties

- Three mirrors (two for beam offset & one for distribution between HED / MID instruments) [1]. Higher harmonics suppression with the mirrors is expected to be in the range of 10⁻⁶.
- Focusing: Be lenses at three positions (229, 857 and 962 m downstream of the undulator exit) resulting in spot sizes of ~200 μ m, ~20 μ m, and 1 – 3 μ m FWHM for 5 – 25 keV [2, 3, 4].
- Split & Delay Line (BMBF project, U Münster): Delays: +/-1 ps (24 keV) to +/-23 ps (5 keV) [7].
- Monochromators: 4-bounce Si₁₁₁ (5 – 25 keV, ~10⁻⁴ Δ E/E) [1], high-resolution monochromator (~10⁻⁶ ∆E/E) [4].

Mirrors, coating B₄C

Focusing concept with CRLs







Top, left: Schematic top view of the six first scientific instruments at European XFEL. Top, right: Pulse picker for HED (rotating disk, 10 Hz). Bottom: Schematic of the electron beam time structure.

Key X-ray beam diagnostics

- In-situ single shot spectrometer combining a diamond grating with a convex Si crystal
- In-situ fast intensity monitors based on back-reflection of diamond foils
- Intensity monitors based on fluorescence screens
- Online monitoring of the arrival time between X-rays and optical lasers







Left: Concept of the single shot spectrometer with technical drawing: the spectrometer crystal can either be used in the direct beam at 10 Hz, or in the full pulse-train using the grating. A intensity monitor for the diffracted beam is available. Right: Technical drawing and picture of the in-situ fast intensity monitor.

X-ray beam transport



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Standardized sample holder concept and load-lock exchange system

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Introduction

The HED instrument focuses on matter at extreme conditions of temperature, pressure, electric and / or magnetic field. The solid sample holder system employs the standardized design concept from the **EUCALL project (proposal #654220)** which consists of a **two-part** system :

(1) inner sample frame standardized outer dimension, and can be modified for specific sample geometry, and

(2) outer carrier frame standardized inner dimension, with unique frame design permanently installed for each facility. The design serves different subsets of user communities to be able to prepare and fabricate samples that are physically compatible at every participating facilities.



Sample monitoring

- Long & short distance cameras to monitor the positioning of the sample
 - ~ 3 out-vacuum cameras (red sqrs position) for long-range view
 - 2-3 in-vacuum cameras (orange sqrs) for high resolution adjustment



Future developments

Motor for high rep-rate (10Hz) experiments
 Scan speed, step-size requirements and limits

 sample dimension (10 x 10 cm^2) limits step-sizes for 10 Hz scanning

fast solid sample scanner

Solid sample loading

- [Above] Load-lock schematic view
 - Gate valve connection to the main interaction chamber (IC)
 - Independent vacuum system to the chamber
 - Positioning of exchanged sample is done with clamps, identification pins & fiducial markers
 - Fast sample scanning x-y motors will be positioned on top of the Hexapod

Sample holder



- Standardized Sample frame & holders
 - (left) Example of the Outer frame.
 - (right) Inner frame, to fit the outer frame. 10cm x 10cm area. Within this dimension, the frame design, geometry and materials can be modified. The sample frame is compatible to those of the ELIMAIA beamline.



- [Below] Sample frame holder cassette
 - Holds up to ~8 samples at a time
 - Sample exchange and refilling without breaking the vacuum nor affecting the setup



Liquid Jet samples

- Liquid jets deliver debris-free samples at repetition rate of 10 Hz [3]
- Using cryogenic liquids provide new materials at solid density such as H₂, He, CH₄, CO₂, ...
- Jets with planar/flat geometries with variable thickness enable controlled dynamic shock compression studies
- Laser driven protons from liquid H₂ jets may be applied for isochoric heating studies
- Development of a platform for routine application of liquid jet techniques at HED under investigation

- Protection from energetic electrons generated from the intense pump dynamics
- Tolerance to EMP from the irradiated targets
- Installation of motor stage cooling system
- EMP tolerance test
 - Planned experiment in Summer 2018 at HiBEF (Institute of Radiaion Physics, Helmholtz-Zentrum Dresden-Rossendorf)
- Sample exchange arm design
 ~ 1 m long foldable mechanism
 Weight tolerance ~ kg.
- C. Deiter et al, EUCALL Grant agreement number: 654220
 I. Prencipe et al., H.P.L.Sci. and Eng. (submitted)





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Status of the Diamond Anvil Setup for the HED instrument of the European XFEL.

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Abstract:

The HED instrument at the European XFEL offers the unique opportunity to develop new experimental capabilities to explore planetary physic of solar and extra solar planets using new static and dynamic DAC x-ray diffraction techniques. Within this poster we describe some of the current ideas to make optimal use of these DACs at the European XFEL and present the current status of the design for a DAC setup for the HED instrument funded within the HIBEF consortium.

Introduction:

Time resolved diffraction at simultaneous high-pressure and -temperatures as well as fast compression/heating is an emerging field in static/dynamic high-pressure physics. This technique may be used to determine Equation of State (EOS) and phase stability at very high pressures and temperatures using the double stage Diamond Anvil Cell (dsDAC, Dubrovinsky et al. 2012) and the dynamic Diamond Anvil Cell (dDAC, Evans et al. 2007), which is not achievable with conventional static high-pressure techniques. In addition one may explore the effects of changing compression rates on the location and kinetics of solid-solid as well as solid-liquid phase transitions using the dynamic Diamond Anvil Cell (dDAC). While dynamic compression diffraction experiments are possible at 3rd generation sources in the kHz (µs) regime, it will require new 4th generation sources, such as the European XFEL, to be able to conduct time resolved experiments in the MHz (ns) regime. Since July of 2015 we have been developing a DAC setup for the "Helmholtz International Beamline for Extreme Fields" (HIBEF) user consortium lead by HZDR and DESY. Below we describe the current status of the design for of the DAC setup to conduct time resolved dynamic compression experiments in the dsDAC and dDAC.





Idea: Perform burst of single shot x-ray diffraction measurements at 4.5 MHz to get EOS of a material in 5 µs (25 bunches) before dsDAC fails.



AGIPD Detector at 4.5 MHz





Fig. 3: Top view of the experimental hutch of the HED instrument with two interaction areas (IA1 and IA2). Located in IA2 is the 2nd interaction chamber (IC2) for either DAC work or standardized shock compression work with the High-Energy Dipole laser. The IC2 sits on a rail system and can be placed at the side of the HED hutch The IA2 may also be used for pulse magnetic field studies or other sample environments.

Design of the Interaction Chamber 2 (IC2) housing the DAC setup at the HED instrument





Second-stage

Time (µs)

Fig. 1 Left: Schematic description of the double stage setup used by Dubrovinsky et al. (2012). Right: Conceptual experimental setup for conducting dsDAC experiments and laser heating using a 1 us laser heating pulse and the 4.5 MHz repetition mode of the XFEL for collecting diffraction images. One may collect 25 diffraction images over approximately 6 us of material response. The material response does not take into account the effect of isochoric heating when using a very small x-ray beam (see Fig. 3).

Idea: Perform single shot x-ray diffraction measurements at 0.5 MHz to determine EOS of a compound in one pulse train (600 µs) before diamonds are destroyed by reactive compounds $(H_2, H_2O_1, ...)$.





Double Sided

• Ray tracing => ongoing (Z. Konopkova, HED) • Pulsed Lasers => ordered from DFG funding

- 20 angle limited by DAC opening (45°)
- 2 =+/-45° covers d = 0.648 Å or Q = 9.7 Å⁻¹ @25 keV
- To cover +/-45° opening with a PE or AGIPD SDD = 200mm
- Difficult when DAC in the center => move DAC 300 mm from the center

Design Established At 200 mm SSD:

- Horizontal 2θ = 28.5°,d = 1.008Å, q = 6.23Å⁻¹ - Vertical $2\theta = 32.8^{\circ}$, d = 0.878Å, q = 7.153Å⁻¹

At 150 mm SSD:

60%

40%

0

<u>د</u> 20%

- Horizontal 2θ = 35.8°, d = 0.807Å, q = 7.787Å⁻¹ - Vertical $2\theta = 40.8^{\circ}$, d = 0.711Å, q = 8.831Å⁻¹

GaAs AGIPD

(Adaptive Gain Integrating Pixel Detector)

-Silicon (500um)

-CdTe (500um)

-Ge / GaAs (500um

Photoelectric absorption of X-rays

40 60

X-ray energy (keV)

20



cification: aAs sensor (100 % QE @ 25 keV) ingle photon counting up to $\sim 10^4$ n/pixel/frame ixel 0. 2 x 0.2 mm² pixel size ize: 1024 × 1024 (200 x 200 mm active area) ax frame rate: 4.5 MHz (burst mode) acuum compatible



HELMHOLTZ **RESEARCH FOR GRAND CHALLENGES**

References:

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XFEL Pulses

583 kHz, 1.7 μs)

Laser Heating &

Evans et al. (2007) Rev. Sci. Instrum., 78, 073904.



